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## Ultrafast Spectroscopy of Donor-Acceptor Oligomers for Photo-voltaic Applications

# physikalisches

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Ort: H46

Gemeinsames Kolloquium der  
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In the last ten years, many alternatives relying on organic molecules have been explored for complementing traditional solar cell technologies relying on inorganic semiconductors. Organic cells are thin, flexible, and cheap-to-produce, but suffer from inherent limitations of organic materials, in particular their low carrier mobility and high exciton binding energies. Nevertheless, the record power conversion efficiency recently reported is as high as 10% [1] for a single junction solar cell.

Solar cells using liquid crystal (LC) films of donor-acceptor (DA) molecules are a new approach, in which the ratio of DA interface-to-volume is maximized, leading to fairly good performances [2-4]. The motivation is to make the distance to the D-A interface shorter than the exciton diffusion length (typically 10 nm). We have studied LC films of bithiophene-derivatives forming D and perylenendiimide as A, by femtosecond transient absorption (TA) spectroscopy. Due to the strong electronic coupling between D's the initial laser excitation, selectively tuned in the absorption of D, excites a coherent superposition of many D molecules (exciton) that decays within 60 fs into a charge transfer (CT) state, that localizes on a slower 0.4 ps time scale [3]. Simulating the quantum kinetics of these intermolecular excitons highlights the dominance of nearest neighbour CT states due to the specific molecular arrangement in the LCs [5].

We will present results obtained for a new type of donor family incorporated in the DA's that bear moieties with different electron-donating and -accepting character, thereby offering a handle to control the localization of HOMO and LUMO orbitals. CT lifetimes larger than 2 ns are now observed in chloroform, and with unexpectedly large effects of the solvent polarity. Simulations of the electronic structure and of intramolecular reorganisation energies find a particular interplay of two CT states of different dipole moments. Results are confronted with a description within Marcus theory.

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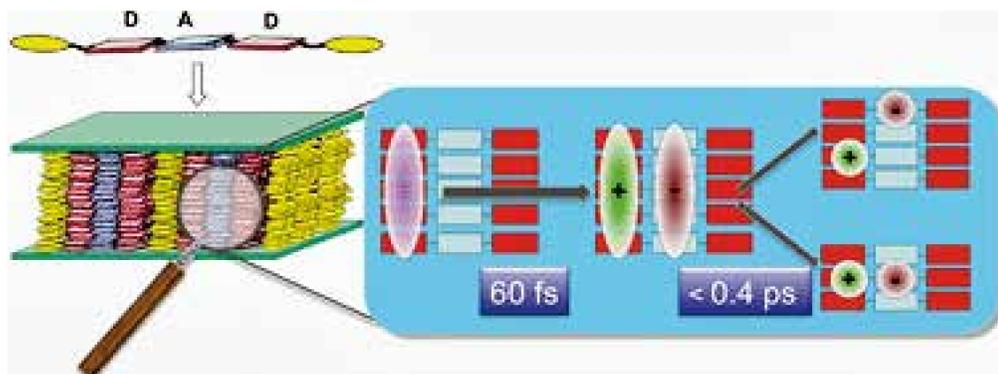
[1] Heliatek press release, [http://www.heliatek.com/newscenter/latest\\_news/](http://www.heliatek.com/newscenter/latest_news/), January 16, 2013; J. Subbiah et al., Adv. Mat. 2015, 27, 702-705; L. Huo, et al., Adv Mat., 2015, 27, 2938.

[2] L. Bu and al., J. Am. Chem. Soc., 2009, 131, 13242-13243

[3] T. Roland and al., Phys. Chem. Chem. Phys., 2012, 14, 273-279

[4] P.O. Schwartz et al., 2014, 136, 5981-92.

[5] M. Polkehn et al., in preparation.



Above: In a liquid-crystal film of D-A oligomers, the intra-molecular spatial coherence leads to ultrafast formation of delocalised CT states within 60 fs, that subsequently localise due to loss of spatial coherence.